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Using first-principles calculations we have predicted new functional properties of oxide ferroic heterostructures. One class of heterostructures utilizes an ultrathin ferroelectric film serving as a barrier between two metal electrodes which makes a ferroelectric tunnel junction (FTJ). The electric-field-induced polarization reversal of the ferroelectric is predicted to have a profound effect on the conductance of the junction leading to a new kind of electroresistive switches. Another class of devices extends functional properties of the FTJs by replacing normal metal electrodes by ferromagnetic which makes the junctions multiferroic. The interplay between ferroelectric and ferromagnetic properties of the two ferroic constituents affects the spin polarization of the tunneling current. Thus, multiferroic tunnel junctions (MFTJ) may provide a new degree of freedom in functionality of magnetoresistive devices.
Also we have explored new possibilities to control the interface magnetization of a magnetic film by an adjacent ferroelectric layer.

15. SUBJECT TERMS
We have predicted new functional properties of oxide ferroic heterostructures and have explored new possibilities to control the interface magnetization of a magnetic film.

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Modeling of Electroresistive and Magnetoelectric Oxide Heterostructures: Final Report

Using first-principles calculations we have predicted new functional properties of oxide ferroic heterostructures. One class of heterostructures utilizes an ultrathin ferroelectric film serving as a barrier between two metal electrodes which makes a ferroelectric tunnel junction (FTJ). The electric-field-induced polarization reversal of the ferroelectric is predicted to have a profound effect on the conductance of the junction leading to a new kind of electroresistive switches. Another class of devices extends functional properties of the FTJs by replacing normal metal electrodes by ferromagnetic which makes the junctions multiferroic. The interplay between ferroelectric and ferromagnetic properties of the two ferroic constituents affects the spin polarization of the tunneling current. Thus, multiferroic tunnel junctions (MFTJ) may provide a new degree of freedom in functionality of magnetoresistive devices.

We have performed first-principles calculation of $SrRuO_3/BaTiO_3/SrRuO_3$ MFTJs which exhibit an tunneling electroresistance (TER) effect associated with the change in the electric polarization of $BaTiO_3$. We demonstrated that the reversal of the electric polarization in $BaTiO_3$ produces a notable change in the conductance, provided that the two interfaces have different terminations. Since $SrRuO_3$ is ferromagnetic, we demonstrated that the $SrRuO_3/BaTiO_3/SrRuO_3$ FTJs exhibit a sizable tunneling magnetoresistance (TMR) effect which is sensitive to the polarization orientation of the ferroelectric spacer layer. Thus, we have proven that these MFTJs may serve as four-state resistance devices. These results reveal the exciting prospects of MFTJs for application as multifunctional spintronic devices.

Also we have explored new possibilities to control the interface magnetization of a magnetic film by an adjacent ferroelectric layer. We have performed first-principles calculations of the magnetoelectric effect at $Fe_3O_4/BaTiO_3$ interfaces. We found that the magnetoelectric coupling in this system originates from the interface bonding sensitive to atomic displacements at the interface. This leads to the change in the interface magnetization when the polarization of the ferroelectric layer reverses. We considered two types of interface terminations of Fe_3O_4 which have different iron cation valence and oxygen atom environment. We found that the magnitude of the magnetoelectric coupling is stronger for the oxygen-deficient $Fe_3O_4/BaTiO_3$ interface. The sensitivity to the interface oxygen content suggests that oxidation or oxygen vacancies at the interface may play an important role in determining the strength of the interface magnetoelectric coupling.

As a result of this work one paper was published and another one was submitted for publication:

1. M. K. Niranjan, J. P. Velev, C.-G. Duan, S. S. Jaswal and E. Y. Tsymbal, "Magnetoelectric effect at the $Fe_3O_4/BaTiO_3$ (001) interface: A first-principles study", *Physical Review B* 78, 104405 (2008).

2. J. P. Velev, C.-G. Duan, J. D. Burton, A. Smogunov, M.K. Niranjan, E. Tosatti, S. S. Jaswal, and E. Y. Tsymbal , "Magnetic tunnel junctions with ferroelectric barriers: Prediction of four resistance states from first-principles", submitted for publication.